Methyl alpha-D-glucopyranoside 97-30-3 | DTXSID7026605

97-	3U-3	ΙD	IVO	וט ו	026	505	

Model Performance

Model	Data

Weighted KNN model

5-fold CV (7	5-fold CV (75%)		75%)	Test (25%	Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

Model Results

Predicted value: 4.92e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.72e-01

Confidence level: 6.84e-01

Nearest Neighbors from the Training Set

Image not found

Endothal

Measured: 5.37e-01 Predicted: 4.10e-01 Image not found
Dexpanthenol

Measured: 4.87 Predicted: 3.46

Image not found

Ethanediamide, N1,N2-bis(2-

hydroxyethyl)-Measured: 7.72e-01 Predicted: 7.57e-01